Recent Results in Charged-Composite Particle Scattering

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Abstract

A brief overview is given of some recent advances in charged-composite particle scattering. On the theoretical side, I address the three-charged particle wave function asymptotics, the nonperturbative investigation of the long-range behaviour of the optical potential, and the question of the compactness of the kernels of the momentum space integral equations for three charged particles. Among the more practical developments, I report on results of numerical calculations of so-called "triangle" amplitudes, a new, simple and very efficient higher-energy approximation for the latter, and a breakthrough in the quantitative treatment of Coulomb effects in proton-deuteron elastic scattering with realistic nuclear potentials.

1 Theoretical Developments

1.1 Asymptotic wave function for three free charged particles

Knowledge of the asymptotic boundary condition on the three-free charged particle wave function is required not only when attempting to solve the Schrödinger equation above the ionization threshold, but also when investigating asymptotic properties of various interesting quantites like the optical potential or the behaviour of the kernel of momentum space integral equations. I, therefore, start by briefly recapitulating some important aspects of the asymptotic behaviour of the solutions of the Schrödinger equation.

Consider three distinguishable particles with masses m_ν and charges e_ν, $\nu = 1, 2, 3$. I use Jacobi coordinates: $\mathbf{k}_\alpha\,(\mathbf{r}_\alpha)$ are relative momentum (coordinate) between particles β and γ, $\mathbf{q}_\alpha\,(\boldsymbol{\rho}_\alpha)$ the relative momentum (coordinate) between particle α and the center of mass of the pair $(\beta\gamma)$. The on-shell momenta are denoted by $(\bar{\mathbf{k}}_\alpha, \bar{\mathbf{q}}_\alpha)$ so that the on-shell relation reads as $E = \bar{q}_\alpha^2/2M_\alpha + \bar{k}_\alpha^2/2\mu_\alpha$, with $\mu_\alpha = m_\beta m_\gamma/(m_\beta + m_\gamma)$ and $M_\alpha = m_\alpha(m_\beta+m_\gamma)/(m_\alpha+m_\beta+m_\gamma)$ being the appropriate reduced masses. Furthermore, $V_\alpha = V_\alpha^S + V_\alpha^C$ is the short-range plus Coulomb potential acting between particles β and γ, and $\bar{\eta}_\alpha \equiv \eta_\alpha(\bar{k}_\alpha) = e_\beta e_\gamma \mu_\alpha/\bar{k}_\alpha$ the corresponding Coulomb parameter. Additional notation: $E_+ = E + i0$, $\epsilon_{\alpha\beta} = -\epsilon_{\beta\alpha} = +1$ if (α, β) = cyclic ordering of (1,2,3); finally, unit vectors are characterised by a hat: $\hat{\mathbf{k}} = \mathbf{k}/k$.

The asymptotic solutions of the Schrödinger equation for three asymptotically free particles in the various regions of configuration space are known:
In Ω_0: $r_1, r_2, r_3 \;\to\; \infty$, but *not* $r_\nu/\rho_\nu \to 0$ for $\nu = 1, 2, 3$ (Redmond, as cited in Ref. [1]):

$$\Psi^{(+)}_{\bar{\mathbf{k}}_\alpha \bar{\mathbf{q}}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) \;\;\approx\;\; e^{i(\bar{\mathbf{k}}_\alpha\cdot\mathbf{r}_\alpha + \bar{\mathbf{q}}_\alpha\cdot\boldsymbol{\rho}_\alpha)} \prod_{\nu=1}^{3} e^{i\bar{\eta}_\nu \ln(\bar{k}_\nu r_\nu - \bar{\mathbf{k}}_\nu\cdot\mathbf{r}_\nu)}. \tag{1}$$

In Ω_α: $\rho_\alpha \to \infty$, $r_\alpha/\rho_\alpha \to 0$, for $\alpha = 1, 2$ or 3 ([2], with some refinements given in [3, 4]):

$$\Psi^{(+)}_{\bar{\mathbf{k}}_\alpha \bar{\mathbf{q}}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) \approx \psi^{(+)}_{\bar{\mathbf{k}}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha)\, e^{i\bar{\mathbf{q}}_\alpha\cdot\boldsymbol{\rho}_\alpha} \prod_{\nu\neq\alpha} e^{i\bar{\eta}_\nu \ln(\bar{k}_\nu \rho_\alpha - \epsilon_{\alpha\nu}\bar{\mathbf{k}}_\nu\cdot\boldsymbol{\rho}_\alpha)}. \tag{2}$$

Here, $\psi^{(+)}_{\bar{\mathbf{k}}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha)$ is continuum solution of the two-body-like Schrödinger equation

$$\left\{\frac{\bar{k}^2_\alpha(\boldsymbol{\rho}_\alpha)}{2\mu_\alpha} + \frac{\Delta_{\mathbf{r}_\alpha}}{2\mu_\alpha} - V_\alpha(\mathbf{r}_\alpha)\right\} \psi^{(+)}_{\bar{\mathbf{k}}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha) = 0, \tag{3}$$

describing the relative motion of particles β and γ with *local* energy $E_\alpha(\boldsymbol{\rho}_\alpha) = \bar{k}^2_\alpha(\boldsymbol{\rho}_\alpha)/2\mu_\alpha$, where (e.g. $\lambda_\beta = \mu_\alpha/m_\gamma$, with $\beta, \gamma \neq \alpha$)

$$\bar{\mathbf{k}}_\alpha(\boldsymbol{\rho}_\alpha) = \bar{\mathbf{k}}_\alpha + \frac{\mathbf{a}_\alpha(\hat{\boldsymbol{\rho}}_\alpha)}{\rho_\alpha}, \quad \mathbf{a}_\alpha(\hat{\boldsymbol{\rho}}_\alpha) = -\sum_{\nu\neq\alpha} \bar{\eta}_\nu \lambda_\nu \frac{\epsilon_{\alpha\nu}\hat{\boldsymbol{\rho}}_\alpha - \hat{\bar{\mathbf{k}}}_\nu}{1 - \epsilon_{\alpha\nu}\hat{\boldsymbol{\rho}}_\alpha \cdot \hat{\bar{\mathbf{k}}}_\nu}. \tag{4}$$

Its parametric dependence on $\boldsymbol{\rho}_\alpha$ is a manifestation of long-ranged three-body correlations; thus it is, in fact, a three-body wave function, the influence of the third particle α however being confined to a shift of the relative momentum of particles β and γ from its asymptotic (for $\rho_\alpha \to \infty$, i.e. particle α is infinitely far apart) value $\bar{\mathbf{k}}_\alpha$ to the *local* value $\bar{\mathbf{k}}_\alpha(\boldsymbol{\rho}_\alpha)$.

1.2 Long-Range Behaviour of the Optical Potential in a Three-Body System

Elastic scattering processes with (charged) composite particles of the type $\alpha + (\beta,\gamma)_m \to \alpha + (\beta,\gamma)_m$ can formally be described by means of a single one-channel LS equation for the elastic scattering amplitude

$$\mathcal{T}_{\alpha m,\alpha m}(z) = \mathcal{V}^{opt}_{\alpha m,\alpha m}(z) + \mathcal{V}^{opt}_{\alpha m,\alpha m}(z)\frac{1}{z - \mathbf{Q}^2_\alpha/2M_\alpha + \hat{E}_{\alpha m}}\mathcal{T}_{\alpha m,\alpha m}(z), \tag{5}$$

where the plane wave matrix elements of the optical potential (OP) operator are given as

$$\begin{aligned}\mathcal{V}^{opt}_{\alpha m,\alpha m}(\mathbf{q}'_\alpha, \mathbf{q}_\alpha; z) &= \langle \mathbf{q}'_\alpha | \langle \psi_{\alpha m} | \bar{V}_\alpha + \bar{V}_\alpha Q_{\alpha m} G(z) Q_{\alpha m} \bar{V}_\alpha | \psi_{\alpha m}\rangle | \mathbf{q}_\alpha \rangle \\ &= \underbrace{\mathcal{V}^{stat}_{\alpha m,\alpha m}(\mathbf{q}'_\alpha, \mathbf{q}_\alpha)}_{\text{static potential}} + \underbrace{\tilde{\mathcal{V}}^{opt}_{\alpha m,\alpha m}(\mathbf{q}'_\alpha, \mathbf{q}_\alpha; z)}_{\text{nonstatic part of OP}} \quad .\end{aligned} \tag{6}$$

The following notation is used: $|\psi_{\alpha m}\rangle$ denotes the target bound state wave function to binding energy $\hat{E}_{\alpha m}$; $G(z) = (z - H_0 - \sum_\nu V_\nu)^{-1}$ and $G^C(z) = (z - H_0 - \sum_\nu V^C_\nu)^{-1}$ are the resolvents of the full and the pure Coulomb three-body Hamiltonian, and $G_\alpha(z) = (z - H_0 - V_\alpha)^{-1}$ the one of the channel Hamiltonian. $P_{\alpha m} = |\psi_{\alpha m}\rangle\langle\psi_{\alpha m}|$ projects onto the target state, and $Q_{\alpha m} = 1 - P_{\alpha m}$ onto the orthogonal complement. Furthermore, $\bar{V}_\alpha = \bar{V}^S_\alpha + \bar{V}^C_\alpha = \sum_{\nu\neq\alpha} V_\nu$ is the channel interaction; $\mathbf{Q}_\alpha$ is the momentum operator with eigenvalue $\mathbf{q}_\alpha$.

The question of solvability of (5) depends on the singular behaviour of $\mathcal{V}^{opt}_{\alpha m,\alpha m}$ in the limit that the momentum transfer $\boldsymbol{\Delta}_\alpha = \mathbf{q}'_\alpha - \mathbf{q}_\alpha$ goes to zero. In leading order, the latter is caused by the Coulombic part $\bar{V}^C_\alpha$ of the channel interaction, i.e., it does not depend on either the short-range part $\bar{V}^S_\alpha$ or on the internal interaction V_α. Of course, a certain behaviour of the optical potential for $\Delta_\alpha \to 0$ implies a corresponding asymptotic behaviour in coordinate space.

As is well known, the static potential has, in the limit $\Delta_\alpha \to 0$, only the trivial Coulomb-type singular behaviour, which for a spherically symmetric target looks like:

$$\mathcal{V}^{stat}_{\alpha m,\alpha m}(\mathbf{q}'_\alpha, \mathbf{q}_\alpha) \overset{\bar{\Delta}_\alpha \to 0}{=} \frac{4\pi e_\alpha(e_\beta + e_\gamma)}{\Delta_\alpha^2} \quad \Longleftrightarrow \quad \mathcal{V}^{stat}_{\alpha m,\alpha m}(\boldsymbol{\rho}_\alpha) \overset{\rho_\alpha \to \infty}{=} \frac{e_\alpha(e_\beta + e_\gamma)}{\rho_\alpha}. \tag{7}$$

The behaviour of the nonstatic OP has been known for a long time, but only in 2^{nd} order perturbation theory which in the present language is equivalent to approximating in (6) the three-body (G) by the channel resolvent (G_α), or in adiabatic approximation. On the energy shell and below the ionisation threshold one has (with $\bar{\boldsymbol{\Delta}}_\alpha = \bar{\mathbf{q}}'_\alpha - \bar{\mathbf{q}}_\alpha$)

$$\tilde{\mathcal{V}}^{opt\,(2)}_{\alpha m,\alpha m}(\bar{\mathbf{q}}'_\alpha, \bar{\mathbf{q}}_\alpha; E_+) \overset{\bar{\Delta}_\alpha \to 0}{\sim} \bar{\Delta}_\alpha \qquad \Longleftrightarrow \qquad \tilde{\mathcal{V}}^{opt\,(2)}_{\alpha m,\alpha m}(\boldsymbol{\rho}_\alpha) \overset{\rho_\alpha \to \infty}{\approx} -\frac{a}{2\rho_\alpha^4}. \tag{8}$$

Here, a is the so-called static dipole polarisability of the composite particle. Two questions arise immediately:
(i) Does the fundamental result (8) hold also for the exact nonstatic OP, i.e., even after all terms of the perturbation expansion of $G(z)$ are summed up? (For $E < 0$, this has been answered in the affirmative, though not fully rigorously, in [5].)
(ii) Does it hold also for $E > 0$? (Within perturbative approaches the answer was yes, but with an energy-dependent "a" in [6], and with the standard a in [7].)

The behaviour of $\tilde{\mathcal{V}}^{opt}_{\alpha m,\alpha m}$ for $\Delta_\alpha \to 0$ has been investigated in [8] nonperturbatively and for all energies, by inserting the spectral decomposition of $G^C(E_+)$ with both two- and three-body intermediate states; for the latter the asymptotic three-charged particle wave function in Ω_α has been used. Off the energy shell we find:

$$\tilde{\mathcal{V}}^{opt}_{\alpha m,\alpha m}(\mathbf{q}'_\alpha, \mathbf{q}_\alpha; E) \overset{\Delta_\alpha \to 0}{=} C_1 \Delta_\alpha + o\,(\Delta_\alpha), \tag{9}$$

with

$$C_1 = -\frac{\pi^2}{4}\left\{ \sum_{n \neq m} \frac{\left[|\mathbf{D}_{nm}|^2 + |\hat{\boldsymbol{\Delta}}_\alpha \cdot \mathbf{D}_{nm}|^2\right]}{[E_+ - q_\alpha^2/2M_\alpha - \hat{E}_{\alpha n}]} + \int \frac{d\mathbf{k}^0_\alpha}{(2\pi)^3} \frac{\left[|\mathbf{D}_{\mathbf{k}^0_\alpha m}|^2 + |\hat{\boldsymbol{\Delta}}_\alpha \cdot \mathbf{D}_{\mathbf{k}^0_\alpha m}|^2\right]}{[E_+ - q_\alpha^2/2M_\alpha - {k^0_\alpha}^2/2\mu_\alpha]} \right\}, \tag{10}$$

and ($N_\alpha = \epsilon_{\alpha\beta} e_\alpha \mu_\alpha [e_\gamma/m_\gamma - e_\beta/m_\beta]$)

$$\mathbf{D}_{nm} = N_\alpha \int d\mathbf{r}_\alpha \psi^*_{\alpha n}(\mathbf{r}_\alpha)\mathbf{r}_\alpha \psi_{\alpha m}(\mathbf{r}_\alpha), \quad \mathbf{D}_{\mathbf{k}^0_\alpha m} = N_\alpha \int d\mathbf{r}_\alpha \psi^{(+)*}_{\mathbf{k}^0_\alpha}(\mathbf{r}_\alpha)\mathbf{r}_\alpha \psi_{\alpha m}(\mathbf{r}_\alpha). \tag{11}$$

On the energy shell, $\tilde{\mathcal{V}}^{opt}_{\alpha m,\alpha m}$ is seen to depend on the momenta only via $\bar{\boldsymbol{\Delta}}_\alpha$, and no longer on the energy. Hence, in coordinate space it is a local, energy-independent potential

$$\tilde{\mathcal{V}}^{opt}_{\alpha m,\alpha m}(\boldsymbol{\rho}_\alpha) \overset{\rho_\alpha \to \infty}{=} -\frac{a}{2\rho_\alpha^4} + o\left(\frac{1}{\rho_\alpha^4}\right), \tag{12}$$

with the polarisability as known from the perturbative approaches:

$$a = 2\sum_{n \neq m} \frac{|\hat{\boldsymbol{\rho}}_\alpha \cdot \mathbf{D}_{nm}|^2}{\left[|\hat{E}_{\alpha m}| - |\hat{E}_{\alpha n}|\right]} + 2\int \frac{d\mathbf{k}^0_\alpha}{(2\pi)^3} \frac{|\hat{\boldsymbol{\rho}}_\alpha \cdot \mathbf{D}_{\mathbf{k}^0_\alpha m}|^2}{\left[|\hat{E}_{\alpha m}| + {k^0_\alpha}^2/2\mu_\alpha\right]}. \tag{13}$$

That is, no "renormalisation" of a arises from the higher order terms in the perturbation expansion of $G(z)$, and all dependence on E which is present in the off-shell "strength factor" $C_1(E)$ has disappeared. Note that along the same lines the existence of a new nonrelativistic contribution to $\tilde{\mathcal{V}}^{opt}_{\alpha m,\alpha m} \sim 1/\rho^5$ has been established recently in [9].

1.3 Compactness properties of the kernels of momentum space integral equations for three charged particles

Three-body integral equations of the Faddeev type can not be used for Coulomb-like potentials, because of the occurrence of singularities in their kernels which destroy the compactness properties known to exist for short-range interactions. Up to now, only for energies below the breakup threshold had attempts been successful to obtain integral equations with compact kernels, by singling out from the original kernel the so-called two-particle Coulomb singularity, in a form such that it could be inverted explicitly [10].

To investigate the behaviour of the kernels for positive energies, we use the rigorously equivalent formulation in terms of an effective-two-body theory [11]. Here, the transition amplitudes for all binary processes satisfy a closed set of coupled LS-type equations

$$\mathcal{T}_{\beta n,\alpha m}(z) = \mathcal{V}_{\beta n,\alpha m}(z) + \sum_{\nu=1}^{3} \sum_{r,s} \mathcal{V}_{\beta n,\nu r}(z)\mathcal{G}_{0;\nu,rs}(z)\,\mathcal{T}_{\nu s,\alpha m}(z). \tag{14}$$

Without loss of generality, the short-range potentials can be taken as separable potentials: $V_\alpha^S = \sum_m |\chi_{\alpha m}\rangle\lambda_{\alpha m}\langle\chi_{\alpha m}|$. The effective potential matrix elements are given as

$$\mathcal{V}_{\beta n,\alpha m}(\mathbf{q}'_\beta, \mathbf{q}_\alpha; z) = \langle \mathbf{q}'_\beta, \chi_{\beta n}|\; G^C(z) - \delta_{\beta\alpha} G_\alpha^C(z)\; |\chi_{\alpha m}, \mathbf{q}_\alpha\rangle. \tag{15}$$

The effective propagator matrix has simple poles in its diagonal for those m which correspond to bound states: $\mathcal{G}_{0;\alpha,mm}(\mathbf{q}_\alpha; z) \sim 1/(z - q_\alpha^2/2M_\alpha - \hat{E}_{\alpha m})$. Note that as a result of our choice of the form of V_α^S, these expressions contain only pure Coulombic quantities.

Define $D_0(z) = z - k_\beta'^2/2\mu_\beta - q_\beta'^2/2M_\beta = z - k_\alpha^2/2\mu_\alpha - q_\alpha^2/2M_\alpha$, with $k'_\beta = |\mathbf{q}_\alpha + \mu_\beta \mathbf{q}'_\beta/m_\gamma|$, $k_\alpha = |\mathbf{q}'_\beta + \mu_\alpha \mathbf{q}_\alpha/m_\gamma|$, $\eta_\beta \equiv \eta_\beta(k'_\beta)$ and $\eta_\alpha \equiv \eta_\alpha(k_\alpha)$. Then, we have now proved [12] that even for positive energies, provided all three particles have charges of equal sign, the leading singularity of the nondiagonal off-shell effective potential is a branch point at $D_0(z) = 0$:

$$\mathcal{V}_{\beta n,\alpha m}(\mathbf{q}'_\beta, \mathbf{q}_\alpha; z) \overset{D_0(z)\to 0}{\sim} 1/D_0(z)^{(1+i\eta_\beta+i\eta_\alpha)}, \;\text{ for } \beta \neq \alpha. \tag{16}$$

This compares with the simple pole occurring in the 'pole' amplitude $\mathcal{V}^{pole}_{\beta n,\alpha m}(\mathbf{q}'_\beta, \mathbf{q}_\alpha; z) = \bar{\delta}_{\beta\alpha}\langle \mathbf{q}'_\beta, \chi_{\beta n}|\; G_0(z)\; |\chi_{\alpha m}, \mathbf{q}_\alpha\rangle \sim 1/D_0(z)$. On the energy shell, it goes over into

$$\mathcal{V}_{\beta n,\alpha m}(\bar{\mathbf{q}}'_\beta, \bar{\mathbf{q}}_\alpha; E_+) \overset{\bar{D}_0\to 0}{\sim} 1/\bar{D}_0^{(1-\eta_{\alpha m}^{(bs)}-\eta_{\beta n}^{(bs)})}, \;\text{ for } \beta \neq \alpha, \tag{17}$$

where we have defined the bound state Coulomb parameter via $\eta_{\alpha m}^{(bs)} = e_\beta e_\gamma \mu_\alpha/\kappa_{\alpha m}$, with $\kappa_{\alpha m}^2 = 2\mu_\alpha|\hat{E}_{\alpha m}|$, and similarly for $\eta_{\beta n}^{(bs)}$, and denoted by $\bar{D}_0 = \bar{k}_\alpha^2/2\mu_\alpha + |\hat{E}_{\alpha m}|$ the on-shell restriction of $D_0(z)$. Since neither the pole nor the branch point singularity can coincide, for real values of the momenta, with the effective propagator pole, both are harmless.

Preliminary results indicate that the diagonal kernels develop on the energy shell a nonintegrable singularity which is, however, of same two-body type ("center-of-mass Coulomb singularity") as that found in [10] for $E < 0$, and in [13, 14] (see also [15]) for all energies within the screening approach; thus, it can be treated by explicit inversion. Apart from that the next strongest singularity occurs off shell and turns out to be $O(\Delta_\alpha^{-5/2})$ for $\Delta_\alpha \to 0$. Thus, it is integrable.

Hence, it appears that after a few iterations the kernels are compact even above the breakup threshold provided the charges of all particles are of equal sign. In contrast, if some of the charges have opposite signs the kernels develop nonintegrable singularities which can destroy the compactness properties.

2 Practical Developments

2.1 Energetic Collisions of Charged Projectiles with Atomic Bound States

Scattering of an elementary charged projectile off a two-charged particle bound state such as hydrogen atoms, positronium, etc., at higher energies can be described by the first few terms of the multiple-scattering expansion of the three-body transition operator:

$$\mathcal{T}_{\beta n,\alpha m}(\bar{\mathbf{q}}'_\beta, \bar{\mathbf{q}}_\alpha) = \langle \bar{\mathbf{q}}'_\beta, \psi_{\beta n}| \{\bar{\delta}_{\beta\alpha} G_0(E_+) + \sum_\nu \bar{\delta}_{\beta\nu}\bar{\delta}_{\nu\alpha} T_\nu^C(E_+) + \cdots\} |\psi_{\alpha m}, \bar{\mathbf{q}}_\alpha\rangle. \tag{18}$$

Here, $G_0(E_+) = (E + i0 - H_0)^{-1}$, T_γ^C the two-body Coulomb T-operator acting between particles α and β, and $\bar{\delta}_{\beta\alpha} = 1 - \delta_{\beta\alpha}$. The momenta satisfy the on-shell condition $E = \bar{q}_\alpha^2/2M_\alpha + \hat{E}_{\alpha m} = \bar{q}_\beta'^2/2M_\beta + \hat{E}_{\beta n}$.

The first ('pole') term of (18) describes the elementary one-particle transfer. The first-order rescattering ('triangle') amplitudes ($\vartheta = \angle(\bar{\mathbf{q}}'_\beta, \bar{\mathbf{q}}_\alpha)$)

$$\sum_\nu \bar{\delta}_{\beta\nu}\bar{\delta}_{\nu\alpha} \langle \bar{\mathbf{q}}'_\beta \mid \langle \psi_{\beta n} \mid T_\nu^C(E+i0) \mid \psi_{\alpha m}\rangle \mid \bar{\mathbf{q}}_\alpha\rangle = \begin{cases} \mathcal{M}^{T^C}_{\beta n,\alpha m}(\vartheta, E) & \text{if} \quad \beta \neq \alpha \\ \sum_{\nu\neq\alpha} \mathcal{M}^{T^C}_{\nu,nm}(\vartheta, E) & \text{if} \quad \beta = \alpha, \end{cases} \tag{19}$$

contribute to both direct ($\beta = \alpha$) and exchange ($\beta \neq \alpha$) scattering. They (as well as all higher-order contributions) contain T^C describing the rescattering of projectile α off each charged target particle. Hence, their calculation is difficult and time-consuming (this is particularly so if the rescattering particles have charges of opposite sign, because of the occurrence of the infinity of bound states). Thus, usually the approximation $T_\nu^C \to V_\nu^C$ is made, yielding the so-called Coulomb-Born Approximation (CBA), to be denoted by $\mathcal{M}^{V^C}_{\beta n,\alpha m}$ and $\mathcal{M}^{V^C}_{\nu,nm}$. But for atomic reactions the CBA is known to fail badly (for attractive and repulsive cases), except for $E \to \infty$ (see [16] and references therein).

We have succeeded to numerically calculate all (direct and exchange) triangle amplitudes for all E and ϑ for arbitrary wave functions, for repulsive and attractive intermediate-state rescattering (for the latter, a 'new' representation of the attractive Coulomb T-matrix for $E < 0$ was developed which has the bound state poles displayed explicitly in a simple, numerically convenient manner). Many concrete results are discussed in [16, 17].

Moreover, we have derived a new approximation in the form of a 'renormalized' CBA:

$$\mathcal{M}^{T^C}_{\gamma,nm}(\vartheta, E) \approx \mathcal{R}^{(s)}_{\gamma,nm}(\vartheta, E)\, \mathcal{M}^{V^C}_{\gamma,nm}(\vartheta, E), \quad \gamma \neq \alpha, \tag{20}$$

$$\mathcal{M}^{T^C}_{\beta n,\alpha m}(\vartheta, E) \approx \mathcal{R}^{(s)}_{\beta n,\alpha m}(\vartheta, E)\, \mathcal{M}^{V^C}_{\beta n,\alpha m}(\vartheta, E), \quad \beta \neq \alpha, \tag{21}$$

with

$$\mathcal{R}^{(s)}_{\gamma,nm}(\vartheta, E) = \frac{A^{i\eta_\gamma^{(d)}}\, \tilde{\mathcal{R}}^{(s)}_{\gamma,nm}(E)}{\Delta_{\alpha\alpha}^{2i\eta_\gamma^{(d)}} \left[\lambda_\alpha^2 \Delta_{\alpha\alpha}^2 + (\kappa_{\alpha n} + \kappa_{\alpha m})^2\right]^{-2i\eta_\gamma^{(d)}}}, \quad \gamma \neq \alpha, \tag{22}$$

$$\mathcal{R}^{(s)}_{\beta n,\alpha m}(\vartheta, E) = \frac{B^{i\eta_\gamma^{(e)}}\, \tilde{\mathcal{R}}^{(s)}_{\beta n,\alpha m}(E)}{\left[\lambda_\beta^2 \Delta_{\beta\alpha}^2 + (\kappa_{\beta n} + \kappa_{\alpha m})^2\right]^{-2i\eta_\gamma^{(e)}}}, \quad \gamma \neq \beta \neq \alpha. \tag{23}$$

Here, the following notation is used: $\mathbf{\Delta}_{\beta\alpha} = \mathbf{q}'_\beta - \lambda_\alpha \mathbf{q}_\alpha/\lambda_\beta$, $\lambda_\alpha = \mu_\alpha/m_\beta$, $\lambda_\beta = \mu_\beta/m_\alpha$; $\kappa_{\alpha m}^2 = 2\mu_\alpha|\hat{E}_{\alpha m}|$ and similarly for $\kappa_{\beta n}^2$. Finally, $\eta_\gamma^{(d,e)} = e_\alpha e_\beta \mu_\gamma/\{2\mu_\gamma(E_+ - k^2_{(d,e)}/2M_\gamma)\}^{1/2}$.

The quantities $k_{(d)}(E), k_{(e)}(E)$ are real, $A(E), B(E)$ are real for $\eta_\gamma^{(d,e)}$ real, and $\tilde{\mathcal{R}}(E)$ is complex. All of them are independent of ϑ, and are explicitly given in terms of simple functions. We note in parentheses that we have also derived approximate analytical expressions for $\mathcal{M}^{V^C}$ (for arbitrary bound state wave functions). When inserted into (21) they yield approximations for the triangle amplitudes containing no quadratures at all (however, their range of validity is somewhat limited). Because of their simple structure, both types are very easy to use for theoretical as well as numerical purposes.

Selected applications: Consider $E > k^2_{(d,e)}/2M_\gamma$ so that $\eta_\gamma^{(d,e)}$ are real. Then ($\mathcal{M}, \tilde{\mathcal{R}}$ without channel indices refer to both 'diagonal' and 'nondiagonal' quantities):
1. The whole ϑ-dependence of $\left|\mathcal{M}^{T^C}\right|$ is given by that of $\left|\mathcal{M}^{V^C}\right|$,

$$\left|\mathcal{M}^{T^C}(\vartheta, E)\right| \approx \left|\tilde{\mathcal{R}}^{(s)}(E)\right| \left|\mathcal{M}^{T^C}(\vartheta, E)\right| : \tag{24}$$

the CBA fails with respect to the magnitude only, insofar as $|\tilde{\mathcal{R}}^{(s)}(E)|$ differs from one.
2. With the penetration factor $C_0^2 = 2\pi\eta_\gamma^{(d,e)}/[\exp\{2\pi\eta_\gamma^{(d,e)}\} - 1]$ pertaining to the intermediate-state Coulomb scattering one finds

$$\left|\mathcal{M}^{T^C}\right| \quad \overset{\eta_\gamma^{(d,e)} \to 0}{=} \quad C_0^2 \left(1 + O(\eta_\gamma^{(d,e)^2})\right) \left|\mathcal{M}^{V^C}\right| \quad \forall\, m, n, \vartheta. \tag{25}$$

Since $C_0^2 < 1 (> 1)$ for $e_\alpha e_\beta > 0 (< 0)$, (25) not only quantifies the charge-sensitivity of $|\mathcal{M}^{T^C}|$ as compared to the insensitivity of $|\mathcal{M}^{V^C}|$ (i.e., $\mathcal{M}^{V^C}(e_\alpha e_\beta > 0) = -\mathcal{M}^{V^C}(e_\alpha e_\beta < 0)$), but it also provides a simple method to quantitatively estimate the former.
3. Since $C_0^2(e_\alpha e_\beta > 0) = C_0^{-2}(e_\alpha e_\beta < 0)\left(1 + O(\eta_\gamma^{(s)2})\right)$ one derives

$$\left|\mathcal{M}^{T^C}_{\gamma,nm}(e_\alpha e_\beta > 0)\right| \left|\mathcal{M}^{T^C}_{\gamma,nm}(e_\alpha e_\beta < 0)\right| \approx \left(\mathcal{M}^{V^C}_{\gamma,nm}\right)^2 \forall\, n, m, \vartheta, E, \tag{26}$$

relating the 'direct' triangle amplitudes for processes with opposite signs of the charges of the rescattering particles.
4. The dependence of $k_{(d,e)}$ on n and m becomes negligible for sufficiently large E, rendering $\eta_\gamma^{(d,e)}$ and C_0^2 practically independent of all bound state characteristics. Consequently, relation (25), and all results derived from it, become universal, i.e., state-independent.

Many numerical tests of the approximate triangle amplitudes have been performed with $e^\pm, p, \bar{p}$ as projectiles and $H, Ps, (\bar{p}, p)$ as targets [16]. Quite generally one finds for both direct and exchange reactions that they reproduce the exact triangle amplitudes already at 1 keV incident energy for light, and at 100 keV for the heavy projectiles, to within a few percent, for practically all scattering angles, the agreement becoming even better with increasing energy. This is to be contrasted with the CBA's: not only are they real, but their magnitudes for light projectiles at 1 keV are off by $\sim$ 40 - 100 per cent, the improvement with increasing energy being slow only. Similarly for heavy projectiles.

2.2 Proton-Deuteron Scattering with Realistic Potentials

Ever since the development of the exact few-body theories, the investigation of the nucleon-deuteron (Nd) elastic scattering and breakup reaction has been at the center of interest, as their principal field of application. For processes with neutrons as projectiles (nd), highly sophisticated calculations are available nowadays, using realistic nuclear potentials including three-body forces. Apart from a few noticeable and as yet unexplained

failures, they provide a good to very good description of all the available observables (for a recent review see [18]). However, experimental nd data are rather sparse and are lacking the desired accuracy. Hence, usually nd calculations are compared with pd data which makes too good an agreement rather questionable.

For proton-induced reactions (pd), on the other hand, data are abundant and of excellent precision, but similarly advanced calculations have hitherto been restricted to $E < 0$ [19, 20] (calculations with simple nuclear potentials, which have been performed for all energies, give in general "only" semiquantitative agreement but they are usually very accurate in explaining observed differences between pd and nd data, see [21, 22] and references therein). The reason for this lack of sophisticated pd calculations above the breakup threshold is obvious: In coordinate space, imposing Coulomb boundary conditions in the whole configuration space is a very difficult task. In momentum space, though the screening and renormalisation approach [13, 14, 15] is in principle straightforward, its application is very computer time consuming (for a pedagogical introduction to the theory and a rather complete list of references, both on theory and calculations, see [15]).

We have now succeeded to obtain for the first time results for cross section and polarisation observables above the breakup threshold for a "realistic" (Paris) potential [23] within the screening and renormalisation approach. In fact, we use a separable representation of the latter (so-called PEST1-6) known to provide an excellent approximation to the original local potential [24]. Up to now the nucleon-nucleon interaction has been taken into account in the states ${}^3S_1 - {}^3D_1$, ${}^1S_0$ and in all P waves. When comparison is made with selected experimental data at 5 and 10 MeV [25, 26], we find good although not perfect agreement of the calculated with measured quantities. Part of the discrepancies (in the polarisation observables A_y and $i\,T_{11}$) exist already in the nd case, implying that there, as well as in our calculations, some aspects of the nuclear force are still missing. Other discrepancies may arise from the restriction in the number of nucleon-nucleon partial waves taken into account, or from a possible influence of the - hitherto neglected - three-body forces. However, the general trends, in particular concerning the relation between neutron and proton data, are well reproduced. Clearly, the observed agreement of nd-calculations with pd-data, in particular for $i\,T_{11}$ and also to a somewhat lesser extent for A_y, is purely fortuitous and does not arise from smallness of Coulomb effects in that observable.

A final remark concerns the fact that we have taken into account the Coulomb interaction in CBA, which for the present case has been estimated in [17, 16] to be accurate to better than 1%.

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